Isotonic regression and isotonic projection *

A. B. Németh
Faculty of Mathematics and Computer Science
Babeş Bolyai University, Str. Kogălniceanu nr. 1-3
RO-400084 Cluj-Napoca, Romania
email: nemab@math.ubbcluj.ro

S. Z. Németh
School of Mathematics, The University of Birmingham
The Watson Building, Edgbaston
Birmingham B15 2TT, United Kingdom
email: nemeths@for.mat.bham.ac.uk

Abstract

The note describes the cones in the Euclidean space admitting isotonic metric projection with respect to the coordinate-wise ordering. As a consequence it is showed that the metric projection onto the isotonic regression cone (the cone defined by the general isotonic regression problem) admits a projection which is isotonic with respect to the coordinate-wise ordering.

1. Introduction

The isotonic regression problem [1, 2, 6, 7, 11, 13, 16] and its solution is intimately related to the metric projection into a cone of the Euclidean vector space. In fact the isotonic regression problem is a special quadratic optimization problem. It is desirable to relate the metric projection onto a closed convex set to some order theoretic properties of the projection itself, which can facilitate the solution of some problems. When the underlying set is a convex cone, then the most natural is to consider the order relation defined by the cone itself. This approach gives rise to the notion of the isotonic projection cone, which by definition is a cone with the metric projection onto it isotonic with respect to the order relation endowed by the cone itself. As we shall see, the two notions of isotonicity, the first related to the regression problem and the second to the metric projection, are at the

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first sight rather different. The fact that the two notions are in fact intimately related (this relation constitute the subject of this note) is somewhat accidental and it derives from semantical reasons.

The relation of the two notions is observed and taken advantage in the paper [3]. There was exploited the fact that the totally ordered isotonic regression cone is an isotonic projection cone too.

The problem occurs as a particular case of the following more general question: *How does a closed convex set in the Euclidean space which admits a metric projection isotonic with respect to some vectorial ordering on the space look like?*

It turns out, that the problem is strongly related to some lattice-like operations defined on the space, and in particular to the Euclidean vector lattice theory. ([8]) When the ordering is the coordinate-wise one, the problem goes back in the literature to [4,9,10,14, 15]. However, we shall ignore these connections in order to simplify the exposition. Thus, the present note, besides proving some new results, has the role to bring together some previous results and to present them in a simple unified form.

2. Preliminaries

Denote by $\mathbb{R}^m$ the m-dimensional Euclidean space endowed with the scalar product $\langle \cdot, \cdot \rangle : \mathbb{R}^m \times \mathbb{R}^m \to \mathbb{R}$, and the Euclidean norm $\|.\|$ and topology this scalar product defines.

Throughout this note we shall use some standard terms and results from convex geometry (see e.g. [12]).

Let K be a *convex cone* in $\mathbb{R}^m$, i. e., a nonempty set with (i) $K + K \subset K$ and (ii) $tK \subset K$, $\forall\, t \in \mathbb{R}_+ = [0, +\infty)$. The convex cone K is called *pointed*, if $K \cap (-K) = \{0\}$. The cone K is *generating* if $K - K = \mathbb{R}^m$. K is generating if and only if $\operatorname{int} K \neq \emptyset$.

A closed, pointed generating convex cone is called *proper*.

For any $x, y \in \mathbb{R}^m$, by the equivalence $x \leq_K y \Leftrightarrow y - x \in K$, the convex cone K induces an *order relation* $\leq_K$ in $\mathbb{R}^m$, that is, a binary relation, which is reflexive and transitive. This order relation is *translation invariant* in the sense that $x \leq_K y$ implies $x + z \leq_K y + z$ for all $z \in \mathbb{R}^m$, and *scale invariant* in the sense that $x \leq_K y$ implies $tx \leq_K ty$ for any $t \in \mathbb{R}_+$. Conversely, if $\preceq$ is a translation invariant and scale invariant order relation on $\mathbb{R}^m$, then $\preceq = \leq_K$ with $K = \{x \in \mathbb{R}^m : 0 \preceq x\}$ a convex cone. If K is pointed, then $\leq_K$ is *antisymmetric* too, that is $x \leq_K y$ and $y \leq_K x$ imply that $x = y$. Conversely, if the translation invariant and scale invariant order relation $\preceq$ on $\mathbb{R}^m$ is also antisymmetric, then the convex cone $K = \{x \in \mathbb{R}^m : 0 \preceq x\}$ is also pointed. (In fact it would be more appropriate to call the reflexive and transitive binary relations preorder relations and the reflexive transitive and antisymmetric binary relations partial order relations. However, for simplicity of the terminology we decided to call both of them order relations.)

The set

$$K = \operatorname{cone}\{x_1, \dots, x_m\} := \{t^1 x_1 + \dots + t^m x_m : \ t^i \in \mathbb{R}_+, \ i = 1, \dots, m\}$$

with $x_1, \dots, x_m$ linearly independent vectors is called a *simplicial cone*. A simplicial cone is closed, pointed and generating.

The *dual* of the convex cone K is the set

$$K^* := \{y \in \mathbb{R}^m : \langle x, y\rangle \geq 0, \ \forall\, x \in K\},$$

with $\langle \cdot, \cdot \rangle$ the standard scalar product in $\mathbb{R}^m$.

The cone K is called *self-dual*, if $K = K^*$. If K is self-dual, then it is a generating, pointed, closed convex cone.

In all that follows we shall suppose that $\mathbb{R}^m$ is endowed with a Cartesian reference system with the standard unit vectors $e_1, \dots, e_m$. That is, $e_1, \dots, e_m$ is an orthonormal system of vectors in the sense that $\langle e_i, e_j\rangle = \delta_i^j$, where δ_i^j is the Kronecker symbol. Then, $e_1, \dots, e_m$ form a basis of the vector space $\mathbb{R}^m$. If $x \in \mathbb{R}^m$, then

$$x = x^1 e_1 + \cdots + x^m e_m$$

can be characterized by the ordered m-tuple of real numbers $x^1, \dots, x^m$, called *the coordinates of* x with respect the given reference system, and we shall write $x = (x^1, \dots, x^m)$. With this notation we have $e_i = (0, \dots, 0, 1, 0, \dots, 0)$, with 1 in the i-th position and 0 elsewhere. Let $x, y \in \mathbb{R}^m$, $x = (x^1, \dots, x^m)$, $y = (y^1, \dots, y^m)$, where x^i, y^i are the coordinates of x and y, respectively with respect to the reference system. Then, the scalar product of x and y is the sum $\langle x, y\rangle = \sum_{i=1}^m x^i y^i$.

The set

$$\mathbb{R}^m_+ = \{x = (x^1, \dots, x^m) \in \mathbb{R}^m : \ x^i \geq 0, \ i = 1, \dots, m\}$$

is called the *nonnegative orthant* of the above introduced Cartesian reference system. A direct verification shows that $\mathbb{R}^m_+$ is a self-dual cone. The order relation $\leq_{\mathbb{R}^m_+}$ induced by $\mathbb{R}^m_+$ is called *coordinate-wise ordering.*

Besides the non-negative orthant, given a Cartesian reference system, the important class of *isotonic regression cones* should be mentioned. Let $w^i > 0$, $i = 1, \dots, m$ be weights and $(V = \{1, \dots, m\}, E)$ be a directed graph of vertices V and edges $E \subset V \times V$ and without loops (a so called *simple directed graph*). (If $(i, j) \in E$, then i is called its *tail*, j is called its *head.*) Then we shall call the set

$$K_E^w = \left\{ x \in \mathbb{R}^m : \ \frac{x^i}{\sqrt{w^i}} \leq \frac{x^j}{\sqrt{w^j}}, \ \forall (i, j) \in E \right\}$$

the *isotonic regression cone defined by the relations E and the weights w^i.*

If (V, E) is connected directed simple graph for which each vertex is the tail respective a head of at most one edge, then K_E^w is called *weighted monotone cone.* In this case K_E^w can be written (after a possible permutation of the standard unit vectors) in the form

$$K_E^w = \left\{ x \in \mathbb{R}^m : \ \frac{x^1}{\sqrt{w^1}} \leq \frac{x^2}{\sqrt{w^2}} \leq \cdots \leq \frac{x^m}{\sqrt{w^m}} \right\}.$$

A *hyperplane* (through $b \in \mathbb{R}^m$) is a set of form

$$H(a, b) = \{x \in \mathbb{R}^m : \ \langle a, x\rangle = \langle a, b\rangle, \ a \neq 0\}. \tag{1}$$

The nonzero vector a in the above formula is called *the normal* of the hyperplane.

A hyperplane $H(a,b)$ determines two *closed half-spaces* $H_-(a,b)$ and $H_+(a,b)$ of $\mathbb{R}^m$, defined by

$$H_-(a,b) = \{x \in \mathbb{R}^m : \langle a, x\rangle \leq \langle a, b\rangle\},$$

and

$$H_+(a,b) = \{x \in \mathbb{R}^m : \langle a, x\rangle \geq \langle a, b\rangle\}.$$

The cone $K \subset \mathbb{R}^m$ is called *polyhedral* if it can be represented in the form

$$K = \cap_{k=1}^n H_-(a_k, 0). \tag{2}$$

If $\operatorname{int} K \neq \emptyset$, and the representation (2) is irredundant, then $K \cap H(a_k, 0)$ is an $m-1$-dimensional convex cone ($k = 1, \dots, n$) and is called a *facet of* K.

The simplicial cone and the isotonic regression cones are polyhedral.

3. Metric projection and isotonic projection sets

Denote by P_D the projection mapping onto a nonempty closed convex set $D \subset \mathbb{R}^m$, that is the mapping which associate to $x \in \mathbb{R}^m$ the unique nearest point of x in D ([17]):

$$P_D x \in D, \ \text{ and } \ \|x - P_D x\| = \inf\{\|x - y\| : \ y \in D\}.$$

Given an order relation $\preceq$ in $\mathbb{R}^m$, the closed convex set is said an *isotonic projection set* if from $x \preceq y, \ x, \ y \in \mathbb{R}^m$, it follows $P_D x \preceq P_D y$.

If $\preceq = \leq_K$ for some cone K, then the isotonic projection set D is called *K-isotonic.*

If the cone K is K-isotonic then it is called an *isotonic projection cone.*

For $K = \mathbb{R}^m_+$ we have $P_K x = x^+$ where x^+ is the vector formed with the non-negative coordinates of x and 0-s in place of negative coordinates. Since $x \leq_K y$ implies $x^+ \leq_K y^+$, it follows that $\mathbb{R}^m_+$ is an isotonic projection cone.

We have the following geometric characterization of a closed, generating isotonic projection cones (Theorem 1 and Corollary 1 in [3]):

Theorem 1 *The closed generating cone $K \subset \mathbb{R}^m$ is an isotonic projection cone if and only if its dual K^* is a simplicial cone in the subspace it spans generated by vectors with mutually non-acute angles.*

4. The nonnegative orthant and its isotonic projection subcones

If $\mathbb{R}^m_+$ is the nonnegative orthant of a Cartesian system, then we have the following theorem (Corollaries 1 and 3 in [8]):

Theorem 2 *Let C be a closed convex set with nonempty interior of the coordinate-wise ordered Euclidean space $\mathbb{R}^m$. Then, the following assertions are equivalent:*

(i) *The projection P_C is $\mathbb{R}^m_+$-isotonic;*

(ii)
$$C = \cap_{i\in\mathbb{N}} H_-(a_i, b_i), \tag{3}$$
where each hyperplane $H(a_i, b_i)$ is tangent to C and the normals a_i are nonzero vectors $a_i = (a_i^1, \dots, a_i^m)$ with the properties $a_i^k a_i^l \le 0$ whenever $k \ne l$, $i \in \mathbb{N}$.

Example 1 *Consider the space $\mathbb{R}^3$ endowed with a Cartesian reference system, and suppose*
$$K_1 = H_-((-2,1,0),0) \cap H_-((1,-2,0),0) \cap H_-((0,0,-1),0),$$
and
$$K_2 = H_-((-2,1,0),0) \cap H_-((1,-2,0),0) \cap H_-((0,1,-1),0).$$
Then K_1 and K_2 are simplicial cones in $\mathbb{R}^3_+$, $x = (1,1,2) \in \operatorname{int} K_i$, $i = 1,2$. Since
$$K_1 = \operatorname{cone}\{(-2,1,0),(1,-2,0),(0,0,-1)\}^\perp$$
and
$$K_2 = \operatorname{cone}\{(-2,1,0),(1,-2,0),(0,1,-1)\}^\perp,$$
using the main result in [5] we see that K_1 is itself an isotonic projection cone, while K_2 is not. Obviously, K_1 and K_2 are both $\mathbb{R}^3_+$-isotonic projection sets.

Example 2 *Let us consider the space $\mathbb{R}^3$ endowed with a Cartesian reference system.*

Consider the vectors
$$a_1 = (-2,1,0),\ a_2 = (1,-2,0),\ a_3 = (-2,0,1),\ a_4 = (1,0,-2),\ a_5 = (0,-2,1),$$
$$a_6 = (0,1,-2).$$
Then,
$$K = \cap_{i=1}^6 H_-(a_i, 0) \subset \mathbb{R}^3_+$$
is by Theorem 2 an $\mathbb{R}^3_+$-isotonic projection cone with six facets.

Indeed, $\langle a_1, x\rangle \le 0$ and $\langle a_2, x\rangle \le 0$ imply that $x^1 \ge 0$ and $x^2 \ge 0$. We can similarly show that $x \in K$ yields $x^3 \ge 0$. Thus, $K \subset \mathbb{R}^3_+$. For $y = (1,1,1)$ we have $\langle a_i, y\rangle < 0$. Hence $y \in \operatorname{int} K$. It follows that K is a proper cone and the sets $H(a_i, 0) \cap K$, $i = 1, \dots, 6$ are different facets of K.

Next we shall show that the cone in Example 2 is in some sense extremal among the $\mathbb{R}^3_+$-isotonic subcones in $\mathbb{R}^3_+$. More precisely we have

Theorem 3 *If K is a generating cone in $\mathbb{R}^m$, then it is $\mathbb{R}^m_+$-isotonic, if and only if it is a polyhedral cone of the form*

$$K = \cap_{k<l}(H_-(a_{kl1}, 0) \cap H_-(a_{kl2}, 0)), \;\; k,\, l \in \{1, \dots, m\} \tag{4}$$

where a_{kli} are nonzero vectors with $a^k_{kli} a^l_{kli} \leq 0$ and $a^j_{kli} = 0$ for $j \notin \{k, l\}$, $i = 1, 2$. Hence K possesses at most $m(m-1)$ facets. There exists a cone K of the above form with exactly $m(m-1)$ facets.

Proof.

The sufficiency is an immediate consequence of Theorem 2. Next we prove the necessity. Assume that K is an $\mathbb{R}^m_+$-isotonic generating cone. By using the same Theorem 2, we have that

$$K = \cap_{i\in\mathcal{J}} H_-(a_i, 0), \tag{5}$$

where $\mathcal{J} \subset \mathbb{N}$ is a set of indices and where each hyperplane $H(a_i, 0)$ is tangent to K and the normals a_i are nonzero vectors $a_i = (a^1_i, \dots, a^m_i)$ with the properties $a^k_i a^l_i \leq 0$ whenever $k \neq l$, $i \in \mathbb{N}$.

First of all we introduce the notation

$$\mathcal{A}_{kl} = \{i : a^j_i = 0,\, j \notin \{k, l\}\}, \;\; k,\, l \in \{1, \dots, m\},\; k < l.$$

(In Example 2 $\mathcal{A}_{12} = \{1, 2\}$, $\mathcal{A}_{13} = \{3, 4\}$, $\mathcal{A}_{23} = \{5, 6\}$.)

We claim that

$$\mathcal{A}_{kl} \neq \emptyset,\; k < l, \text{ and } \cup_{k<l} \mathcal{A}_{kl} = \mathcal{J}. \tag{6}$$

This follows from the structure of the normals a_i. Indeed if a_i possesses two non-zero components, say a^k_i and a^l_i, $k < l$, then $i \in \mathcal{A}_{kl}$. If it has only one non-zero component, say a^k_i with $k < m$, then $i \in \mathcal{A}_{km}$, or only one nonzero component a^m_i then $i \in \mathcal{A}_{km}$ for $k < m$.

Let us see that

$$\cap_{i\in\mathcal{A}_{kl}} H_-(a_i, 0) = H_-(a_{i_1}, 0) \cap H_-(a_{i_2}, 0), \tag{7}$$

where $H_-(a_{i_j}, 0)$ are among those in (5) and the case $i_1 = i_2$ is possible.

Denote by $\mathbb{R}_{kl}$ the bidimensional subspace in $\mathbb{R}^m$ endowed by the k-th and l-th axis. Then we have the representation

$$\cap_{i\in\mathcal{A}_{kl}} H_-(a_i, 0) = \mathbb{R}^\perp_{kl} \times (\cap_{i\in\mathcal{A}_{kl}} H_-(a_i, 0)) \cap \mathbb{R}_{kl}.$$

Now, $\cap_{i\in\mathcal{A}_{kl}} H_-(a_i, 0)) \cap \mathbb{R}_{kl}$ must be a two dimensional cone in $\mathbb{R}_{kl}$ (since K is generating), hence it must have one or two extremal rays. That is the intersection can be expressed by one or two terms, that is, we can suppose that $1 \leq \operatorname{card} \mathcal{A}_{kl} \leq 2$ and (7) is proved.

With these remarks we can assert that the formula (5) becomes

$$K = \cap_{k<l} (\cap_{i\in\mathcal{A}_{kl}} H_-(a_i, 0)) = \cap_{k<l}(H_-(a_{kl1}, 0) \cap H_-(a_{kl2}, 0)), \tag{8}$$

where $a^k_{kli} a^l_{kli} \leq 0$ and $a^j_{kli} = 0$ for $j \notin \{k, l\}$, $i = 1, 2$.

From formula (8) it follows that in the representation (5) of K there are at most $m(m-1)$ facets $H(a_i,0)\cap K$ of K.

Using the construction in Example 2 we can construct a K with exactly $m(m-1)$ facets. To this end, let for $k<l$ a_{kl1} be the vector with $a^k_{kl1}=-2,\quad a^l_{kl1}=1$ and $a^j_{kl1}=0$ for $j\notin\{k,l\}$, and a_{kl2} be the vector with $a^k_{kl2}=1,\quad a^l_{kl2}=-2$ and $a^j_{kl2}=0$ for $j\notin\{k,l\}$. We have that the vectors a_{kli} are pairwise non-parallel. Putting these vectors in the representation (8) we get a proper subcone of $\mathbb{R}^m_+$ which is $\mathbb{R}^m_+$-isotonic and possesses exactly $m(m-1)$ facets. Indeed, we must see that in this case the representation (8) is irredundant. But this follows from the fact that $K\subset\mathbb{R}^m_+$ is a polyhedral cone with $x=(1,1,\dots,1)$ an interior point. Hence some of $F_{kli}=H(a_{kli},0)\cap K$ must be facets of K. Now, from the special feature of a_{kli} it follows that the sets F_{kli} are structurally equivalent and if one of them is a facet, then all of them are so.

The proof also implies that K must be a polyhedral cone and if its representation (5) is irredundant, than the set $\mathcal{J}$ must be finite.

$\square$

Remark 1 *The representation (8) can be redundant, even if the original one in (5) is irredundant. Indeed, $\mathbb{R}^m_+$ must be of form (5) and its irredundant representation contains m terms, while its equivalent form (8) formally contains much more terms. In this case (8) can contain $\frac{m(m-1)}{2}$ terms. But even a minimal "dual" decomposition of $\mathbb{R}^m_+$ is of cardinality $[\frac{m+1}{2}]$ and hence it contains $2[\frac{m+1}{2}]$ half-spaces.*

5. Every isotonic regression cone is an $\mathbb{R}^m_+$-isotonic projection set

Projecting $y\in\mathbb{R}^m$ into K given by (8) we have to solve the following quadratic minimization problem:

$$P_Ky=\operatorname{argmin}\left\{\sum_{i=1}^m(x^i-y^i)^2 : a^k_{kl1}x^k+a^l_{kl1}x^l\le 0,\ a^k_{kl2}x^k+a^l_{kl2}x^l\le 0,\ k<l\right\},\qquad (9)$$

where the cases $a^k_{klj}=0$, or $a^l_{klj}=0$ are not excluded.

By using Theorem 2, we see that, from

$$u\le_{\mathbb{R}^m_+}v,$$

it follows that

$$P_Ku\le_{\mathbb{R}^m_+}P_Kv.$$

A particular case of this projection problem is equivalent to the so called *isotonic regression problem* [1, 2, 6, 7, 11, 13, 16] which can be described as follows:

For a given $y \in \mathbb{R}^m$ and weights $w_i > 0$, $i = 1, \dots, m$

$$\operatorname{iso}(y) := \operatorname{argmin}\left\{\sum_{i=1}^{m} w_i (x^i - y^i)^2 : x^i \le x^j,\ \forall (i,j) \in E\right\},$$

where $(V = \{1, \dots, m\}, E)$ is a directed simple graph.

Indeed,

$$\operatorname{iso}(y) = \operatorname{argmin}\left\{\sum_{i=1}^{m} \left(\sqrt{w^i} x^i - \sqrt{w^i} y^i\right)^2 : \frac{\sqrt{w^i} x^i}{\sqrt{w^i}} \le \frac{\sqrt{w^i} x^j}{\sqrt{w^j}},\ \forall (i,j) \in E\right\}$$
$$= \frac{1}{\sqrt{w}} P_{K_E^w}(\sqrt{w} y),$$

where for any $z \in \mathbb{R}^m$ we denote

$$\sqrt{w} z = (\sqrt{w^1} z^1, \dots, \sqrt{w^m} z^m)$$

and

$$\frac{z}{\sqrt{w}} = \left(\frac{z^1}{\sqrt{w^1}}, \dots, \frac{z^m}{\sqrt{w^m}}\right),$$

and K_E^w is the isotonic regression cone defined in Section 2.

To compare with this with the general projection problem (9), we observe that the restrictions on x for $P_{K_E^w}(y)$ are of the form

$$a_{ij}^i x^i + a_{ij}^j x^j \le 0$$

with $a_{ij}^i = 1/\sqrt{w^i}$ and $a_{ij}^j = -1/\sqrt{w^j}$, $(i,j) \in E$. Thus we have established the

Corollary 1 *Every isotonic regression cone K_E^w is an $\mathbb{R}_+^m$-isotonic projection set.*

We further have that

Proposition 1 *The isotonic regression cone K_E^w is an isotonic projection cone if and only if in the oriented graph (V, E) does not exist different edges with same tail or different edges with same head, that is, edges of form (i,j) and (i,k) with $j \neq k$, or edges of form (i,j) and (k,j) with $i \neq k$.*

Proof. Assume e. g. that $(1,2),\ (1,3) \in E$. Then the corresponding normals are

$$a_{1,2} = (1/\sqrt{w^1}, -1/\sqrt{w^2}, 0, \dots, 0)$$

and

$$a_{1,3} = (1/\sqrt{w^1}, 0, -1/\sqrt{w^3}, 0, \dots, 0).$$

Then $a_{1,2}$ and $a_{1,3}$ are normals in the irreducible representation of K_E^w, and $\langle a_{1,2}, a_{1,3}\rangle > 0$. Thus, according to Theorem 1 K_E^w cannot be an isotonic projection cone. Conversely, if there are no vertices with the above type multiplicity property, then the normals in the irreducible representation of K_E^w (which in fact generates $-K_E^{w*}$) form pair-wise non-acute angles, hence by the same result K_E^w is an isotonic projection cone.

$\square$

Corollary 2 *If K_E^w is an isotonic projection cone, then (V, E) splits in disjoint union of connected simple graphs with vertices being the tails or heads of at most one edge. The single (up to a permutation of the canonical basis) isotonic regression cone K_E^w, with (V, E) a directed connected simple graph, which is also an isotonic projection cone is the weighted monotone cone.*

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